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# Molecular understanding of kidney stone management: A focus on molecular ligand-target insight of glycolate oxidase (GOX) inhibitors from a traditional ayurvedic polyherbal formulation

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The objective of present investigation is to search lead molecules from natural products as a part of drug discovery campaigns in the management of kidney stones. We employed modern technologies in finding promiscuous molecules from a treasure of Indian Ayurvedic system of medicine. Inspired by a pending appeal from therapeutic area of kidney stone to add effective drug in its armamentarium, we explored Gokshuradi Yog (GY) formulation, due to its continuous use in kidney stone management by Ayurvedic practitioners. Bioassay guided isolation of leads from individual plant extracts of GY formulation was done by employing GOx from spinach. These bioassay guided leads isolated were characterized and its structures elucidated by analytical techniques. In silico molecular modeling of those molecules was done at active site of GOx and it has revealed potential binding with key amino acid residues conserved within the active site. Antiurolithic activity of the isolated leads was confirmed in an in vivo model of ethylene glycol induced urolithiasis in experimental rats.

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